Asymptotics of the ground state energy for atoms and molecules in the self-generated magnetic field

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1 Problem

sect-1

This is a last in the series of three papers (following [17, 18]) and the theorem 1.1 and corollary 1.2 below constitute the final goal of this series. Arguments of this paper are rather standard; all the heavy lifting was done before. Let us consider the following operator (quantum Hamiltonian)

1-1   (1.1)
$$\mathsf{H} = \sum_{1 \le j \le N} H^0_{x_j} + \sum_{1 \le j < k \le N} |x_j - x_k|^{-1}$$

in

1-2   (1.2)
$$\mathfrak{H} = \bigwedge_{1 \le n \le N} \mathscr{H}, \qquad \mathscr{H} = \mathscr{L}^2(\mathbb{R}^3, \mathbb{C}^2)$$

with

1-3   (1.3)
$$H^0 = \left((i\nabla - A) \cdot \sigma\right)^2 - V(x)$$

Let us assume that

1-4   (1.4) Operator H is self-adjoint on $\mathfrak{H}$.

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We will never discuss this assumption. We are interested in the *ground state energy* $\mathsf{E}_N^*(A)$ of our system i.e. in the lowest eigenvalue of the operator H on $\mathfrak{H}$:

$\boxed{\text{1-5}}$ (1.5)
$$\mathsf{E}_N^*(0) = \inf \operatorname{Spec} \mathsf{H} \qquad \text{on } \mathfrak{H}$$

as $A = 0$ and more generally in

$\boxed{\text{1-6}}$ (1.6)
$$\mathsf{E}_N^* = \inf_A \left(\inf \operatorname{Spec}_{\mathfrak{H}} \mathsf{H} + \frac{1}{\alpha} \int |\nabla \times A|^2 \, dx \right)$$

where

$\boxed{\text{1-7}}$ (1.7)
$$V(x) = \sum_{1 \le m \le M} \frac{Z_m}{|x - x_m|}$$

$\boxed{\text{1-8}}$ (1.8)
$$N \approx Z \gg 1, \qquad Z := Z_1 + \dots Z_M, \qquad Z_1 > 0, \dots, Z_M > 0$$

M is fixed, under assumption

$\boxed{\text{1-9}}$ (1.9)
$$0 < \alpha \le \kappa^* Z^{-1}$$

with sufficiently small constant $\kappa^* > 0$.

Our purpose is to prove

$\boxed{\text{thm-1-1}}$ **Theorem 1.1.** *Under assumption* ($\overset{\text{1-9}}{1.9}$) *as* $N \ge Z - CZ^{-\frac{2}{3}}$

$\boxed{\text{1-10}}$ (1.10)
$$\mathsf{E}_N^* = \mathcal{E}_N^{\mathsf{TF}} + \sum_{1 \le m \le M} 2Z_m^2 S(\alpha Z_m) + O\left(N^{\frac{16}{9}} + \alpha a^{-3} N^2\right)$$

provided

$\boxed{\text{1-11}}$ (1.11)
$$a := \min_{1 \le m < m' \le M} |x_m - x_{m'}| \ge N^{-\frac{1}{3}}$$

where $\mathcal{E}_N^{\mathsf{TF}}$ *is a* Thomas-Fermi *energy (see* $\overset{\text{Lieb-1}}{[\mathrm{L1}]}$ or $\overset{\text{ivrii:ground}}{[\mathrm{IS}]}$*) and* $S(Z_m)Z_m^2$ *are magnetic Scott correction terms (see* $\overset{\text{EFS3}}{[\mathrm{EFS3}]}$ or $\overset{\text{MQT11}}{[8]}$*).*

Combining with the properties of the Thomas-Fermi energy we arrive to

$\boxed{\text{cor-1-2}}$ **Corollary 1.2.** *Let us consider* $x_m = x_m^0$ *minimizing full energy*

$\boxed{\text{1-12}}$ (1.12)
$$\mathsf{E}_N^* + \sum_{1 \le m < m' \le M} Z_m Z_{m'} |x_m - x_{m'}|^{-1}.$$

Assume that

$\boxed{\text{1-13}}$ (1.13)
$$Z_m \asymp N \qquad \forall m = 1, \dots, M.$$

Then $a \ge N^{-\frac{1}{4}}$ *and the remainder estimate in* ($\overset{\text{1-10}}{1.10}$) *is* $O\left(N^{\frac{16}{9}}\right)$.

Remark 1.3. As $\alpha = 0$ the remainder estimate (1.12) was proven in [IS] and the remainder estimate $O\big(N^{\frac{5}{3}}(N^{-\delta} + a^{-\delta})\big)$ in [FS] for atoms ($M = 1$) and [12] for $M \geq 1$; this better asymptotics contains also Dirac and Schwinger correction terms. Unfortunately I was not able to recover such remainder estimate here unless α satisfies stronger assumption than (1.9). I still hope to achieve this better estimate without extra assumptions.

Recall that Thomas-Fermi potential W^{TF} and Thomas-Fermi density ρ^{TF} satisfy equations

(1.14)
$$\rho^{\mathsf{TF}} = \frac{1}{3\pi^2}(W^{\mathsf{TF}})^{\frac{3}{2}}$$

and

(1.15)
$$W^{\mathsf{TF}} = V^0 + \frac{1}{4\pi}|x|^{-1} * \rho^{\mathsf{TF}}.$$

We prove theorem 1.1 in sections 2 "Lower estimate" and 3 "Upper Estimate". Section 4 "Miscellaneous" is devoted to corollary 1.2 and a brief discussion.

2 Lower estimate

Consider corresponding to H quadratic form

(2.1) $\quad \langle \mathsf{H}\Psi, \Psi \rangle = \sum_j (H^0_{x_j}\Psi, \Psi) + \big(\sum_{1 \leq j < k \leq N} |x_j - x_k|^{-1}\Psi, \Psi \big) =$

$$\sum_j (H_{x_j}\Psi, \Psi) + ((V - W)\Psi, \Psi) + \big(\sum_{1 \leq j < k \leq N} |x_j - x_k|^{-1}\Psi, \Psi \big)$$

with

(2.2)
$$H = \big((i\nabla - \mathbf{A}) \cdot \boldsymbol{\sigma}\big)^2 - W(x)$$

where we select W later. By Lieb-Oxford inequality the last term is estimated from below:

(2.3) $\quad \langle \sum_{1 \leq j < k \leq N} |x_j - x_k|^{-1}\Psi, \Psi \rangle \geq \mathsf{D}(\rho_\Psi, \rho_\Psi) - C \int \rho_\Psi^{\frac{4}{3}}\, dx$

where

$\boxed{\text{2-4}}$ (2.4)
$$\rho_\Psi(x) = N \int |\Psi(x; x_2, \ldots, x_N)|^2 \, dx_2 \cdots dx_N$$

is a spatial density associated with Ψ and

$\boxed{\text{2-5}}$ (2.5)
$$D(\rho, \rho') := \frac{1}{2} \iint |x - y|^{-1} \rho(x) \rho'(y) \, dx dy$$

Therefore

$\boxed{\text{2-6}}$ (2.6) $\langle H\Psi, \Psi \rangle \geq$
$$\sum_j (H_{x_j}\Psi, \Psi) - 2((V - W)\Psi, \Psi) + D(\rho_\Psi, \rho_\Psi) - C \int \rho_\Psi^{\frac{4}{3}} \, dx =$$
$$\sum_j (H_{x_j}\Psi, \Psi) - 2D(\rho, \rho_\Psi) + D(\rho_\Psi, \rho_\Psi) - C \int \rho_\Psi^{\frac{4}{3}} \, dx =$$
$$\sum_j (H_{x_j}\Psi, \Psi) - D(\rho, \rho) + D(\rho - \rho_\Psi, \rho - \rho_\Psi) - C \int \rho_\Psi^{\frac{4}{3}} \, dx$$

as

$\boxed{\text{2-7}}$ (2.7)
$$W - V = |x|^{-1} * \rho.$$

Note that due to antisymmetry of Ψ

$\boxed{\text{2-8}}$ (2.8)
$$\sum_j (H_{x_j}\Psi, \Psi) \geq \sum_{1 \leq j \leq N : \lambda_j < 0} \lambda_j \geq \text{Tr}^-(H)$$

where λ_j are eigenvalues of H.

To estimate the last term in (2.6) we reproduce the proof of Lemma 4.3 from [ES3]:

According to magnetic Lieb-Thirring inequality for $U \geq 0$:

$\boxed{\text{2-9}}$ (2.9)
$$\sum_{j \leq N} \langle (H_{x_j}^0 - U)\Psi, \Psi \rangle \geq -C \int U^{5/2} \, dx - C\gamma^{-3} U^4 \, dx - \gamma \int B^2 dx$$

$B = \nabla \times A$, $\gamma > 0$ is arbitrary. Selecting $U = \beta \min(\rho_\Psi^{5/3}, \gamma \rho_\Psi^{4/3})$ with $\beta > 0$ small but independent from γ we ensure $\frac{1}{2} U\rho_\Psi \geq CU^{5/2} + C\gamma^{-3} U^4$ and then

$\boxed{\text{2-10}}$ (2.10)
$$\sum_{j \leq N} \langle (H_{x_j}^0)\Psi, \Psi \rangle \geq \epsilon \int \min(\rho_\Psi^{5/3}, \gamma \rho^{4/3}) dx - \gamma \int B^2 \, dx$$

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which implies

2-11   (2.11) $\displaystyle\int \rho_\Psi^{4/3}\,dx \le \gamma^{-1}\int \min(\rho_\Psi^{5/3}, \gamma\rho^{4/3})\,dx + \gamma\int \rho_\Psi\,dx \le$

$$c\gamma^{-1}\sum_{j:\lambda_j<0}\langle(H_{x_j}^0)\Psi,\Psi\rangle + c\int B^2\,dx + c\gamma N$$

where we use $\int \rho_\Psi\,dx = N$.

rem-2-1   *Remark 2.1.* As one can prove easily (see also [ES3]) that

2-12   (2.12) $\displaystyle\sum_{j\le N}\langle(H_{x_j}^0)\Psi,\Psi\rangle \le CZ^{\frac{4}{3}}N$

we conclude that

2-13   (2.13) $\displaystyle\int \rho_\Psi^{4/3}\,dx \le CZ^{\frac{2}{3}}N + C_1\int B^2\,dx.$

It is sufficient unless we want to recover Dirac-Schwinger terms which unfortunately are too far away for us.

Therefore skipping the non-negative third term in the right-hand expression of (2.6) we conclude that

2-14   (2.14) $\displaystyle\langle H\Psi,\Psi\rangle + \frac{1}{\alpha}\int |\nabla\times A|^2\,dx \ge$

$$\mathrm{Tr}^-(H) + \left(\frac{1}{\alpha} - C_1\right)\int |\nabla\times A|^2\,dx - D(\rho,\rho) - CN^{\frac{5}{3}}.$$

Applying Theorem 5.2 from [18] we conclude that

2-15   (2.15), the sum of the first and the second terms in the right-hand expression of (2.14) is greater than

$$\frac{2}{15\pi^2}\int W^{\frac{5}{2}}\,dx + \sum_m 2Z_m^2 S(\alpha Z_m) - CN^{\frac{16}{9}} - C\alpha a^{-3}N^2.$$

To prove this estimate one needs just to rescale $x \mapsto xN^{\frac{1}{3}}$, $a \mapsto aN^{\frac{1}{3}}$ and introduce $h = N^{-\frac{1}{3}}$ and $\kappa = \alpha N$. Here one definitely needs the regularity properties like in [18] but we have them as $\rho = \rho^{\mathsf{TF}}$, $W = W^{\mathsf{TF}}$. Also one can see easily that "$-C_1$" brings correction not exceeding $C_2 \alpha N^2$ as $\alpha N \leq 1$.

Meanwhile for $\rho = \rho^{\mathsf{TF}}$, $W = W^{\mathsf{TF}}$

(2.16) $$\frac{2}{15\pi^2} \int W^{\frac{5}{2}} \, dx - \mathsf{D}(\rho, \rho) = \mathcal{E}^{\mathsf{TF}}.$$

Lower estimate of Theorem 1.1 has been proven.

Remark 2.2. $\rho = \rho^{\mathsf{TF}}$, $W = W^{\mathsf{TF}}$ delivers the maximum of the right-hand expression of (2.16) among ρ, W satisfying (2.7).

3 Upper Estimate

Upper estimate is easy. Plugging as Ψ the *Slater determinant* (see [IS] f.e.) of $\psi_1, \ldots, \psi_N$ where $\psi_1, \ldots, \psi_N$ are eigenfunctions of $H_{A,W}$ we get

(3.1) $\langle H\Psi, \Psi \rangle = \mathsf{Tr}^-(H_{A,W} - \lambda_N) + \lambda_N N +$
$$\int (W - V)(x)\rho_\Psi(x) \, dx + \mathsf{D}(\rho_\Psi, \rho_\Psi) -$$
$$\frac{1}{2} N(N-1) \iint |x_1 - x_2|^{-1} |\Psi(x_1, x_2; x_3, \ldots, x_N)|^2 \, dx_1 \cdots dx_N$$

where we don't care about last term as we drop it (again because we cannot get sharp enough estimate) and the first term in the second line is in fact

(3.2) $$- 2\mathsf{D}(\rho, \rho_\Psi);$$

provided (2.7) holds. Thus we get

(3.3) $\mathsf{Tr}^-(H_{A,W} - \lambda_N) + \lambda_N N - \mathsf{D}(\rho, \rho) + \mathsf{D}(\rho_\Psi - \rho, \rho_\Psi - \rho) +$
$$\frac{1}{\kappa} \int |\partial A|^2 \, dx$$

where we added magnetic energy. Definitely we have several problems here: λ_N depends on A and there may be less than N negative eigenvalues.

However in the latter case we can obviously replace N by the lesser number $\bar{N} := \max(n \leq N, \lambda_n \leq 0)$ as E_N^* is decreasing function of N. In this case the first term in (3.3) would be just $\mathsf{Tr}^-(H_{A,W})$ and the second would be 0. Then we apply theory of [18] immediately without extra complications.

Consider A a minimizer (or its mollification) for potential $W = W^{\mathsf{TF}}$ and $\mu \leq 0$. Then with an error $O(N^{\frac{2}{3}})$

$$\#\{\lambda_k < \mu\} = \int (W - \mu)_+^{\frac{3}{2}} \, dx + O(N^{\frac{2}{3}}). \tag{3.4}$$

One can prove (3.4) easily using the regularity properties of A established in [18] and the same rescaling as before. Note that the first term in (3.4) differs from the same expression with $\mu = 0$ (which is equal to Z) by $\asymp \mu(N^{4/3})^{1/2} \cdot N^{-1} = \mu N^{-1/3}$. Then as the left-hand expression equals N, and $N - Z = O(N^{\frac{2}{3}})$, we conclude that $|\lambda_N| = O(N)$.

Therefore modulo $O\big(N^{\frac{16}{9}} + \kappa a^{-3} N^2\big)$ the sum of the first and the last term in (3.3) is equal to

$$\frac{2}{15\pi^2} \int (W - \lambda_N)_+^{\frac{5}{2}} \, dx + \sum_m 2Z_m^2 S(\kappa Z_m) \tag{3.5}$$

and modulo $O(N^{-\frac{1}{3}}\lambda_N^2) = O(N^{\frac{5}{3}})$ one can rewrite the first term here as

$$\frac{2}{15\pi^2} \int W_+^{\frac{5}{2}} \, dx - \lambda_N \frac{1}{3\pi^2} \int W_+^{\frac{3}{2}} \, dx \tag{3.6}$$

and with the same error the second term here cancels term $\lambda_N N$ in (3.3); then (3.3) becomes

$$\frac{2}{15\pi^2} \int W_+^{\frac{5}{2}} \, dx + \sum_m 2Z_m^2 S(\kappa Z_m) - \mathsf{D}(\rho, \rho) + \mathsf{D}(\rho_\Psi - \rho, \rho_\Psi - \rho) \tag{3.7}$$

and as $W = W^{\mathsf{TF}}$, $\rho = \rho^{\mathsf{TF}}$ the first and the third term together are $\mathcal{E}^{\mathsf{TF}}$, so we get again $\mathcal{E}^{\mathsf{TF}} + \sum_m 2Z_m^2 S(\kappa Z_m)$.

Now we need to estimate properly the last term in (3.7) i.e.

$$\frac{1}{2} \iint |x - y|^{-1} \big(\rho_\Psi(x) - \rho^{\mathsf{TF}}(x)\big)\big(\rho_\Psi(y) - \rho^{\mathsf{TF}}(y)\big) \, dxdy. \tag{3.8}$$

Rescaling as before, and using (1.14) we conclude that it does not exceed

$$N^{\frac{5}{3}} \iint \varrho(x)^2 \varrho(y)^2 \ell^{-1}(x)\ell^{-1}(y)|x - y|^{-1} \, dxdy \tag{3.9}$$

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where ϱ is ρ of [18] and we know that $\varrho = \ell^{-\frac{1}{2}}$ as $\ell \leq 1$ and $\varrho = \ell^{-2}$ as $\ell \geq 1$.

Estimating integral by the (double) sum of integral as $\ell(x) \leq 1$, $\ell(y) \leq 1$ and $\ell(x) \geq 1$, $\ell(y) \geq 1$ we get (increasing C)

$$C \int_{\{|y| \leq |x| \leq 1\}} |x-y|^{-1}|x|^{-2}|y|^{-2} \, dy dx \asymp 1$$

and

$$C \int_{\{|y| \geq |x| \geq 1\}} |x-y|^{-1}|x|^{-3}|y|^{-3} \, dy dx \asymp 1$$

respectively.

This concludes the proof of the upper estimate in Theorem 1.1 which is proven now.

4   Miscellaneous

sect-4

Proof. Proof of corollary 1.2 Optimization with respect to $x_1, \ldots, x_M$ implies

4-1   (4.1)
$$\mathsf{E}^* < \sum_{1 \leq m \leq M} \mathsf{E}^*_m$$

where $\mathsf{E}^* = \mathsf{E}^*(x_1, \ldots, x_M; Z_1, \ldots, Z_m, N)$ and $\mathsf{E}^*_m = \mathsf{E}^*(Z_m, Z_m)$ are calculated for separate atoms. In virtue of theorem 1.1 and (1.9) then

4-2   (4.2)
$$\mathcal{E}^{\mathsf{TF}} - \sum_{1 \leq m \leq M} \mathcal{E}^{\mathsf{TF}}_m \leq Ca^{-3}N + CN^{\frac{16}{9}};$$

however due to strong non-binding theorem in Thomas-Fermi theory (see f.e. [S]) the left-hand expression is $\asymp a^{-7}$ as $a \geq N^{-\frac{1}{3}}$ and therefore (4.2) implies

4-3   (4.3)
$$a \geq \epsilon_1 N^{-\frac{16}{21}}$$

and $a^{-3}N \leq N^{\frac{16}{9}}$.

On the other hand, there is no binding with $a \leq N^{-\frac{1}{3}}$ because remainder estimate is (better than) CN^2 and binding energy excess is $\asymp N^{\frac{7}{3}}$. $\square$

rem-4-1   *Remark 4.1.* Similar arguments work if we improve $N^{\frac{16}{9}}$ to N^{ν} with $\nu \geq \frac{7}{4}$ but without improving $a^{-3}N$ part of the remainder estimate we would not pass beyond $O(N^{\frac{7}{4}})$.

There are several questions which after [18]$^{\text{MQT11}}$ could be answered in this framework by the standard arguments with certain error but we postpone it, hoping to improve remainder estimate $O(h^{-\frac{4}{3}})$ in [18]$^{\text{MQT11}}$:

`problem-4-2` *Problem 4.2.* (i) Investigate case $N \leq Z - CZ^{\frac{2}{3}}$;

(ii) Estimate from above excess negative charge (how many extra electrons can and bind atom) ionization energy $(E^*_{N-1} - E^*_N)$;

(iii) Estimate from above excess positive charge in the case of binding of several atoms i.e. estimate $Z - N$ as

`4-4` (4.4)
$$E^*(x_1, \ldots, x_M; Z_1, \ldots, Z_m, N) < \min_{\substack{N_1, \ldots, N_m: \\ N_1 + \ldots + N_M = N}} E^*_m(Z_m, N_m).$$

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